

Connecting via Winsock to STN

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LOGINID:SSSPTAAJP1626

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TERMINAL (ENTER 1, 2, 3, OR ?):2

***** Welcome to STN International *****

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 FEB 25 CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS 4 FEB 28 PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS 5 FEB 28 BABS - Current-awareness alerts (SDIs) available
NEWS 6 FEB 28 MEDLINE/LMEDLINE reloaded
NEWS 7 MAR 02 GBFULL: New full-text patent database on STN
NEWS 8 MAR 03 REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS 9 MAR 03 MEDLINE file segment of TOXCENTER reloaded
NEWS 10 MAR 22 KOREAPAT now updated monthly; patent information enhanced
NEWS 11 MAR 22 Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS 12 MAR 22 PATDPASPC - New patent database available
NEWS 13 MAR 22 REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS 14 APR 04 EPFULL enhanced with additional patent information and new fields
NEWS 15 APR 04 EMBASE - Database reloaded and enhanced
NEWS 16 APR 18 New CAS Information Use Policies available online
NEWS 17 APR 25 Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAPLUS and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications.
NEWS 18 APR 28 Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAPLUS

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

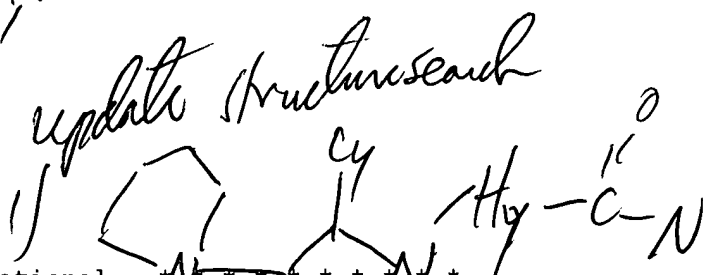
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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***** STN Columbus *****

5/20/05 10/699/106



incomplete search - too many results
N-Hy-C-N
7 but CAPLUS

FILE 'HOME' ENTERED AT 13:40:22 ON 20 MAY 2005

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 13:40:29 ON 20 MAY 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 MAY 2005 HIGHEST RN 850784-62-2

DICTIONARY FILE UPDATES: 19 MAY 2005 HIGHEST RN 850784-62-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

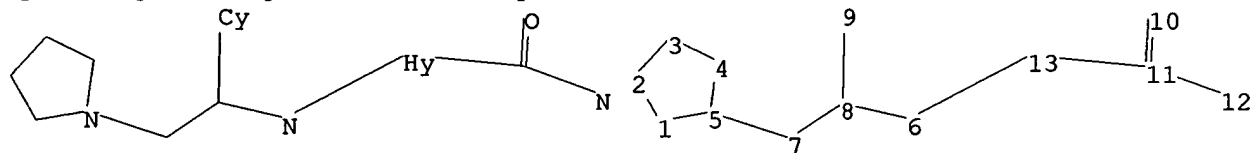
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10699106\10699106e.str



chain nodes :

6 7 8 9 10 11 12 13

ring nodes :

1 2 3 4 5

chain bonds :

5-7 6-8 6-13 7-8 8-9 10-11 11-12 11-13

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 5-7 6-8 6-13 8-9 10-11 11-12 11-13

exact bonds :
7-8

Match level :

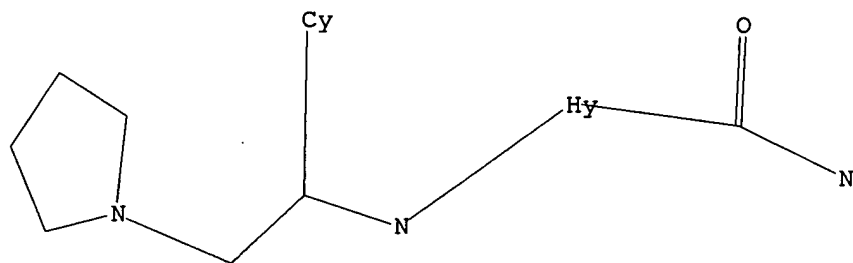
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L1

SAMPLE SEARCH INITIATED 13:40:47 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 34367 TO ITERATE

2.9% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 676264 TO 698416
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 13:40:52 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 687320 TO ITERATE

53.7% PROCESSED 368752 ITERATIONS
58.2% PROCESSED 400000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.23

0 ANSWERS

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 687320 TO 687320
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS FUL L1

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

163.91

164.12

FILE 'REGISTRY' ENTERED AT 13:44:38 ON 20 MAY 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 MAY 2005 HIGHEST RN 850784-62-2

DICTIONARY FILE UPDATES: 19 MAY 2005 HIGHEST RN 850784-62-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

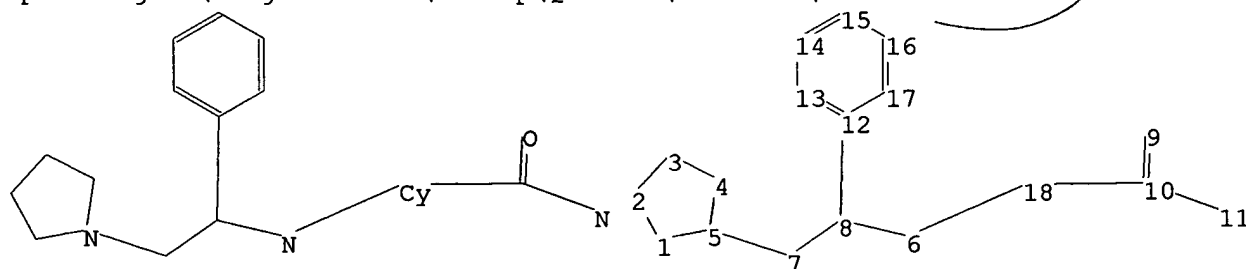
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10699106\10699106f.str



chain nodes :

6 7 8 9 10 11 18

ring nodes :

1 2 3 4 5 12 13 14 15 16 17

chain bonds :

5-7 6-8 6-18 7-8 8-12 9-10 10-11 10-18
 ring bonds :
 1-2 1-5 2-3 3-4 4-5 12-13 12-17 13-14 14-15 15-16 16-17
 exact/norm bonds :
 1-2 1-5 2-3 3-4 4-5 5-7 6-8 6-18 9-10 10-11 10-18
 exact bonds :
 7-8 8-12
 normalized bonds :
 12-13 12-17 13-14 14-15 15-16 16-17

Match level :

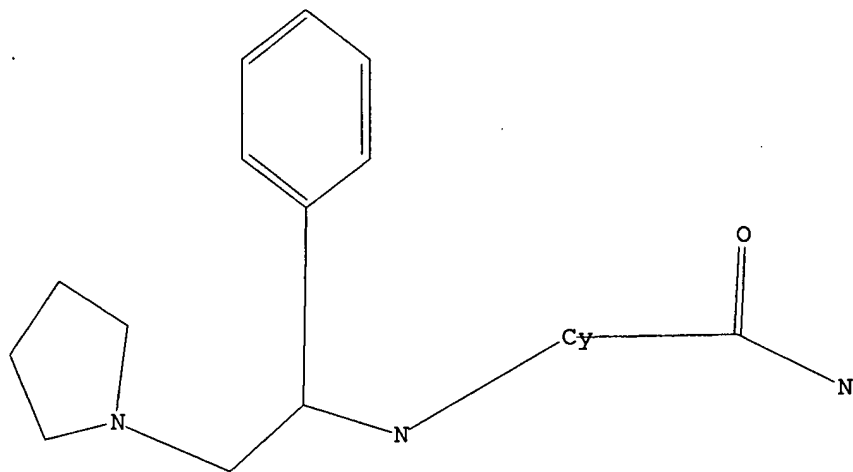
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
 10:CLASS 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L4

SAMPLE SEARCH INITIATED 13:44:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1395 TO ITERATE

71.7% PROCESSED 1000 ITERATIONS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

7 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 25660 TO 30140
 PROJECTED ANSWERS: 8 TO 382

L5 7 SEA SSS SAM L4

=> s L4 full

FULL SEARCH INITIATED 13:45:01 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 27357 TO ITERATE

100.0% PROCESSED 27357 ITERATIONS
SEARCH TIME: 00.00.01

157 ANSWERS

L6 157 SEA SSS FUL L4

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

161.33

325.45

FILE 'CAPLUS' ENTERED AT 13:45:08 ON 20 MAY 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 20 May 2005 VOL 142 ISS 22

FILE LAST UPDATED: 19 May 2005 (20050519/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L6

L7 7 L6

=> d ibib abs hitstr 1-7

L7 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:390231 CAPLUS

DOCUMENT NUMBER: 140:391196

TITLE: Process for the preparation of pyrrolidinyl ethylamine compounds via a copper-mediated aryl amination

INVENTOR(S): Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

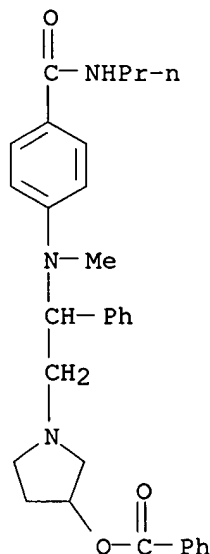
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039785	A1	20040513	WO 2003-IB4676	20031022
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TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 US 2004152896 A1 20040805 US 2003-699106 20031031
 PRIORITY APPLN. INFO.: US 2002-423328P P 20021101
 OTHER SOURCE(S): MARPAT 140:391196
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention provides a new process for the preparation of the well-known kappa agonists I via a copper salt-catalyzed amination of an oxazolidinone II with an aryl halide III in the presence of an amino ligand and a base [wherein A = H, OH and derivs., fluoro/alkyl, etc.; Ar1 = (un)substituted phenyl; Ar2 = (un)substituted Ph, naphthyl, pyridinyl, thiophenyl, furyl, pyrrolyl, pyrimidinyl; R1 = alkyl, benzyl, with its Ph part optionally substituted; R2, R3 = independently H, (un)substituted alkyl, or R2R3N = (un)substituted pyrrolidine, piperidine, morpholine; X = Cl, Br, I]. The advantages of the aryl amination include high yields, mild, efficient, cost-effective and robust process. For example, aryl amination of S-(+)-4-phenyloxazolidin-2-one with 4-bromo-N-propylbenzamide in the presence of CuI/K2CO3 gave the intermediate IV, used in the synthesis of pyrrolidinyl ethylamine V.

IT **686347-77-3P**, Benzoic acid 1-[2-[methyl[4-(propylcarbamoyl)phenyl]amino]-2-phenylethyl]pyrrolidin-3-yl ester
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (amine product; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)
 RN 686347-77-3 CAPLUS
 CN Benzamide, 4-[[2-[3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

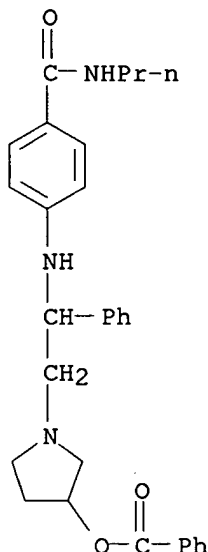


IT **686347-76-2P**, Benzoic acid 1-[2-phenyl-2-[[4-(propylcarbamoyl)phenyl]amino]ethyl]pyrrolidin-3-yl ester

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for preparation of pyrrolidiny ethylamines via a copper-mediated aryl amination)

RN 686347-76-2 CAPLUS

CN Benzamide, 4-[[2-[3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)



L7 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:877272 CAPLUS

DOCUMENT NUMBER: 140:111217

TITLE: Efficient synthesis of the κ -opioid receptor agonist CJ-15,161: four stereospecific inversions at a single aziridinium stereogenic center

AUTHOR(S): Couturier, Michel; Tucker, John L.; Andresen, Brian M.; DeVries, Keith M.; Vanderplas, Brian C.; Ito, Fumitaka

CORPORATE SOURCE: Chemical Research & Development, Pfizer Inc., Groton, CT, 06340, USA

SOURCE: Tetrahedron: Asymmetry (2003), 14(22), 3517-3523
CODEN: TASYE3; ISSN: 0957-4166

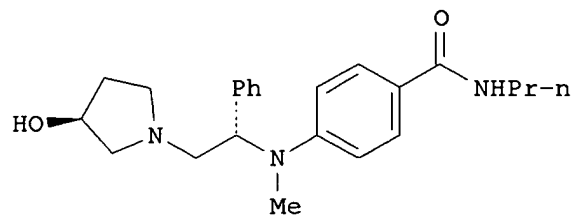
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:111217

GI



I

AB An efficient four-step sequence has been developed for the synthesis of the κ -opioid receptor agonist I (CJ-15,161). The process features four consecutive regioselective and stereospecific inversions at a single aziridinium stereogenic center, which leads to overall retention of stereochem., in a single operation. The chemical is straightforward, practical and amenable to large-scale synthesis. Crystal structure of suitable for formulation polymorph benzoate salt form of I is also reported.

IT **646041-98-7**

RL: PRP (Properties)

(crystal structure; large-scale synthesis of κ -opioid receptor agonist, (arylamino) (phenyl)ethyl pyrrolidinol)

RN 646041-98-7 CAPLUS

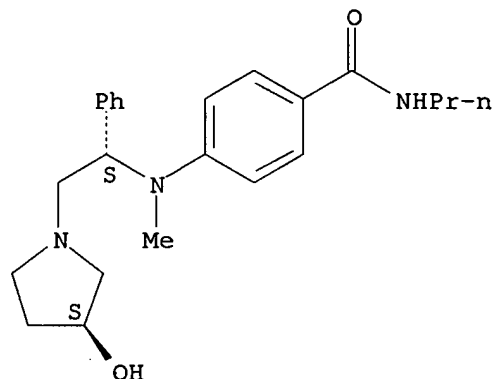
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monobenzoate (salt), monohydrate (9CI) (CA INDEX NAME)

CM 1

CRN 204970-97-8

CMF C23 H31 N3 O2

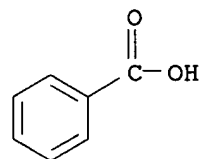
Absolute stereochemistry. Rotation (+).



CM 2

CRN 65-85-0

CMF C7 H6 O2



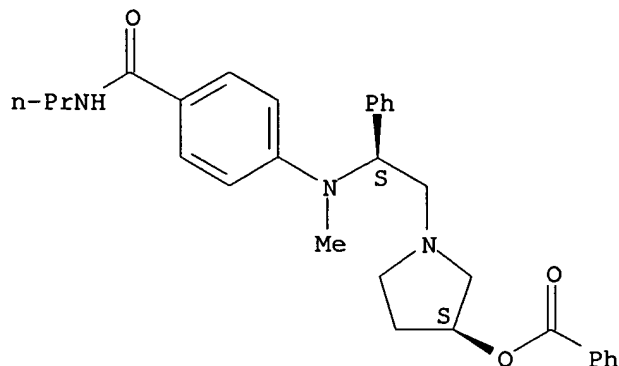
IT **473916-34-6P**

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (large-scale synthesis of κ -opioid receptor agonist, (arylamino) (phenyl)ethyl pyrrolidinol)

RN 473916-34-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 204970-97-8P

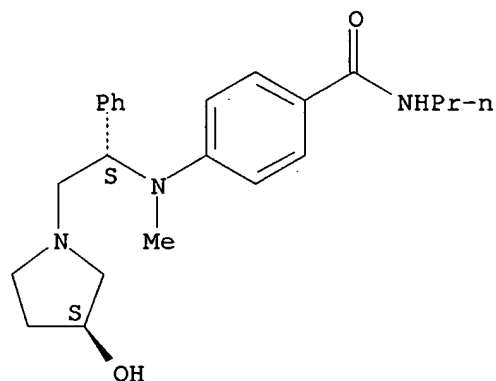
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(large-scale synthesis of κ -opioid receptor agonist, (arylamino)(phenyl)ethyl pyrrolidinol)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:696867 CAPLUS

DOCUMENT NUMBER: 139:230618

TITLE: Preparation of crystalline anhydrous and monohydrate benzoate salts of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine as κ -opioid receptor agonists

INVENTOR(S): Quallich, George Joseph; Castaldi, Michael James

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

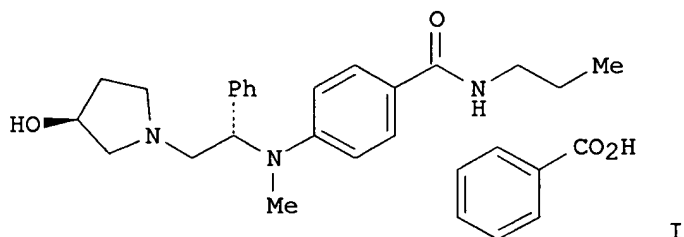
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

after PKOV date

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072544	A1	20030904	WO 2003-IB560	20030217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2477634	AA	20030904	CA 2003-2477634	20030217
EP 1478622	A1	20041124	EP 2003-742880	20030217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003008052	A	20041228	BR 2003-8052	20030217
US 2004235936	A1	20041125	US 2003-421209	20030423
PRIORITY APPLN. INFO.:			US 2002-360250P	P 20020228
			WO 2003-IB560	W 20030217

GI



AB A process for preparing an anhydrous crystalline benzoate salt of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine (I) and the corresponding I crystalline benzoate monohydrate is described which comprises: salifying (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine with benzoic acid in the presence of an alkyl alc. (e.g., 2-propanol), and isolating the anhydrous I salt (X-ray diffraction data is presented). The crystalline monohydrate benzoate salt of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine is prepared by: treating anhydrous I with an aqueous alkanol solution; and isolating the crystallization I monohydrate (X-ray diffraction data is presented). These benzoate salts are selective kappa-receptor agonists, and are useful as analgesics, anesthetics, anti-inflammatory or neuroprotective agents, or in the treatment of arthritis, stroke or functional bowel disease (all no data).

IT 591769-11-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of crystalline anhydrous and monohydrate benzoate salts of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine as κ -opioid receptor agonists)

RN 591769-11-8 CAPLUS

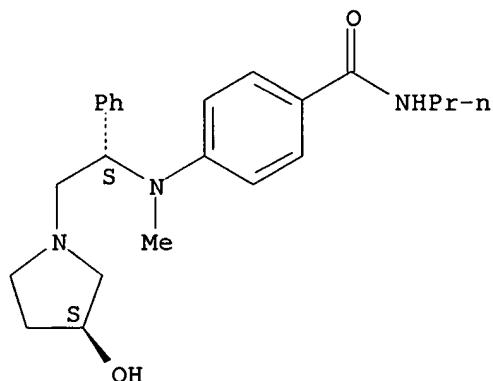
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, compd. with phenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 204970-97-8

CMF C23 H31 N3 O2

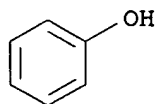
Absolute stereochemistry. Rotation (+).



CM 2

CRN 108-95-2

CMF C6 H6 O



IT 591769-12-9P

RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of crystalline anhydrous and monohydrate benzoate salts of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine as κ -opioid receptor agonists)

RN 591769-12-9 CAPLUS

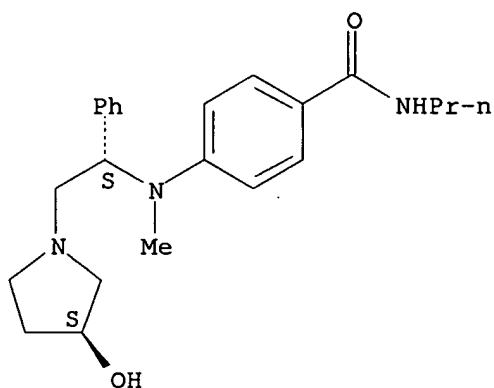
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, compd. with phenol (1:1), monohydrate (9CI) (CA INDEX NAME)

CM 1

CRN 204970-97-8

CMF C23 H31 N3 O2

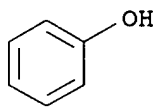
Absolute stereochemistry. Rotation (+).



CM 2

CRN 108-95-2

CMF C6 H6 O



IT 204970-97-8

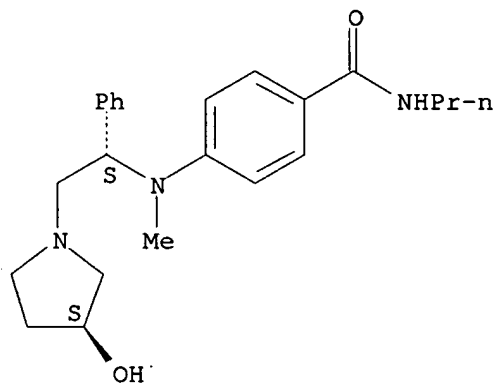
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of crystalline anhydrous and monohydrate benzoate salts of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine as κ -opioid receptor agonists)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:833565 CAPLUS

DOCUMENT NUMBER: 137:337777

TITLE: Preparation of hydroxypyrrolidinyl ethylamine compounds useful as selective κ -opioid receptor agonists

INVENTOR(S): Devries, Keith M.; Couturier, Michel A.; Andresen, Brian M.; Tucker, John L.; Ito, Fumitaka

PATENT ASSIGNEE(S): Pfizer Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 13 pp.
CODEN: USXXCO

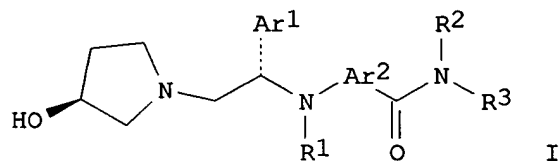
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002161241	A1	20021031	US 2002-133954	20020426
US 6624313	B2	20030923		
CA 2445874	AA	20021107	CA 2002-2445874	20020325
WO 2002088082	A2	20021107	WO 2002-IB924	20020325
WO 2002088082	A3	20040521		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
BR 2002009270	A	20040615	BR 2002-9270	20020325
EP 1461317	A2	20040929	EP 2002-716961	20020325
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
JP 2005508851	T2	20050407	JP 2002-585384	20020325
PRIORITY APPLN. INFO.:			US 2001-287428P	P 20010430
			US 2001-314006P	P 20010821
			WO 2002-IB924	W 20020325
OTHER SOURCE(S):		CASREACT 137:337777; MARPAT 137:337777		
GI				



AB Hydroxypyrrolidinyl ethylamine compds. [I; wherein R1 = H, OH, (C1-C4)alkyl, (C1-C4)alkoxy, etc.; R2, R3, independently = H, (C1-C4)alkyl; Ar1, Ar2, independently = aryl, and particularly phenyl] were prepared. For example, (2'S,3S)-3-benzoyloxy-N-(2-[N-methyl-N-4-(N-propylaminocarbonyl)phenyl]amino-2-phenyl)ethylpyrrolidine was prepared by a multistep synthetic procedure. The compds. are useful as selective κ -opioid receptor agonists. In fact, some of the title compds. showed a potent IC50 value against kappa-receptor in the range of 0.01 to 100 nM.

IT 204970-97-8P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

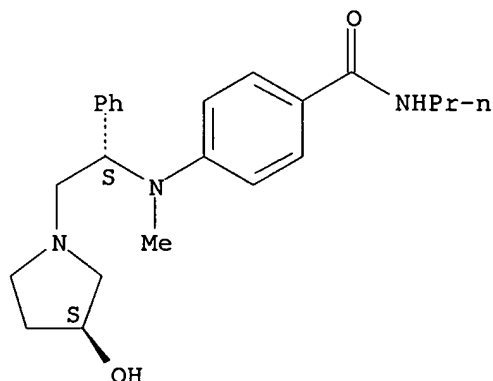
PREP (Preparation); USES (Uses)

(preparation of hydroxypyrrolidinyl ethylamine compds. useful as selective κ -opioid receptor agonists)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 473916-34-6P

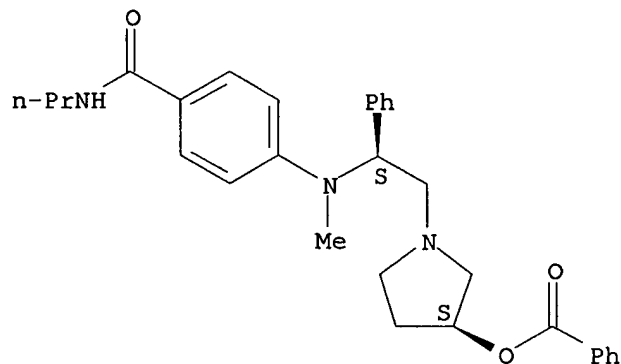
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of hydroxypyrrolidinyl ethylamine compds. useful as selective κ -opioid receptor agonists)

RN 473916-34-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L7 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:517323 CAPLUS

DOCUMENT NUMBER: 138:73134

TITLE: Synthesis of the kappa-agonist CJ-15,161 via a palladium-catalyzed cross-coupling reaction

AUTHOR(S): Ghosh, Arun; Sieser, Janice E.; Caron, Stephane; Watson, Timothy J. N.

CORPORATE SOURCE: Chemical Research and Development, Pfizer Global Research and Development, Groton, CT, 06340-8013, USA

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (15), 1644-1645

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:73134

AB Syntheses of CJ-15,161 involving intermol. N-arylation of an appropriately functionalized diamine, obtained from the precursor α -amino acids or, more conveniently, from the corresponding 1,2-amino alcs. via 1,2,3-oxathiazolidine-2,2-dioxide, are reported.

IT **479687-38-2P**

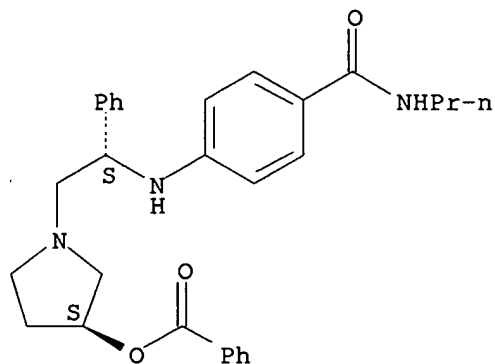
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(formylation of; preparation of kappa-agonist compound via palladium-catalyzed cross-coupling reactions)

RN 479687-38-2 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **473916-34-6P**

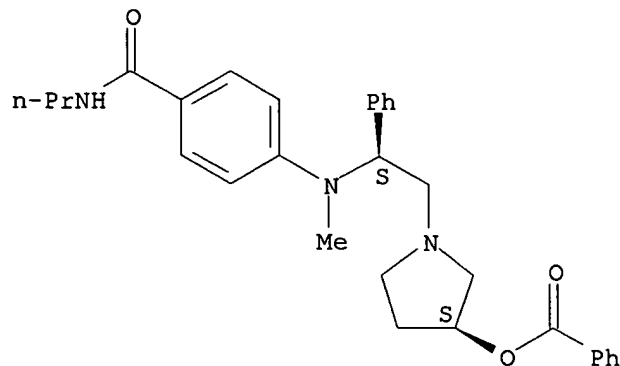
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(hydrolysis of; preparation of kappa-agonist compound via palladium-catalyzed cross-coupling reactions)

RN 473916-34-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 204970-97-8P

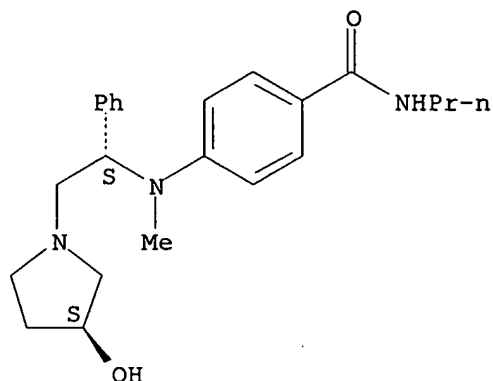
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of kappa-agonist compound via palladium-catalyzed cross-coupling reactions)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:178439 CAPLUS

DOCUMENT NUMBER: 134:222619

TITLE: Preparation of pyrrolidinyl- and pyrrolinylethylarylamines as kappa opioid receptor agonists

INVENTOR(S): Ito, Fumitaka; Kondo, Hiroshi

PATENT ASSIGNEE(S): Pfizer, Inc., USA

SOURCE: U.S., 39 pp., Cont.-in-part of Appl. No. PCT/IB96/00957.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

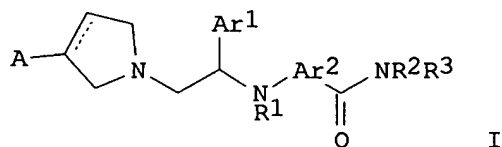
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6201007	B1	20010313	US 1999-254805	19990312
WO 9812177	A1	19980326	WO 1997-IB1021	19970821
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RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
JP 2001316344	A2	20011113	JP 2001-92342	19970821
US 2001008890	A1	20010719	US 2001-770515	20010126
US 6310061	B2	20011030		
US 2001009921	A1	20010726	US 2001-770513	20010126
US 6313302	B2	20011106		
US 2001011091	A1	20010802	US 2001-770514	20010126
US 6294569	B2	20010925		
US 2001014683	A1	20010816	US 2001-771029	20010126

cited in Spec.

discloses compound

US 6307061	B2	20011023		
US 2001020024	A1	20010906	US 2001-771030	20010126
US 6294557	B2	20010925		
US 6303602	B1	20011016	US 2001-770512	20010126
PRIORITY APPLN. INFO.:			WO 1996-IB957	A2 19960918
			WO 1997-IB1021	W 19970821
			JP 1998-514433	A3 19970821
			US 1999-254805	A3 19990312

OTHER SOURCE(S): MARPAT 134:222619
GI



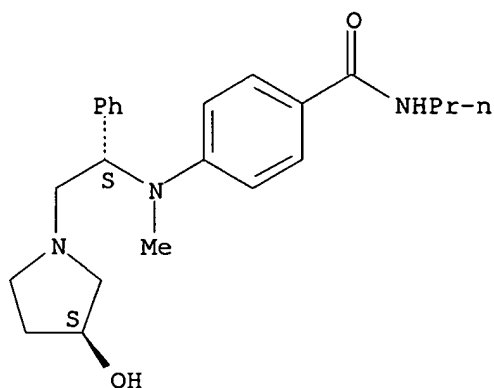
AB Title compds. [I; A = H, halo, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, O, OY, null; Y = protecting group; broken line = optional double bond; Ar1 = (substituted) Ph; Ar2 = (substituted) Ph, naphththyl, pyridyl, thienyl, furyl, pyrrolyl, pyrimidinyl; R1 = H, OH, alkyl, alkoxy, OY; and R2, R3 = (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, alkoxy, Ph, etc.; R2R3N = (substituted) pyrrolidinyl, piperidinyl, morpholinyl], were prepared as κ agonists (no data). Thus, a mixture of 2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethanol, 2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-2-(R)-phenylethanol (preparation given), and Et3N in CH2Cl2 was treated with MeSO2Cl at 0° followed by 5,5 h stirring at room temperature to give a residue which was refluxed 1.5 h with Me 4-methylaminobenzoate in EtOH to give 62.5% Me 4-[N-[2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethyl]-N-methylamino]benzoate. This was saponified with NaOH in MeOH (quant.) and the acid was stirred with PrNH2 and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride in CH2Cl2 to give 72% Me 4-[N-[2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethyl]-N-methylamino]-N'-propylbenzamide.

IT **204970-97-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrrolidinyl- and pyrrolinylethylarylamines as kappa opioid receptor agonists)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT	204970-95-6P	204970-99-0P	204971-01-7P
	204971-03-9P	204971-05-1P	204971-07-3P
	204971-09-5P	204971-11-9P	204971-13-1P
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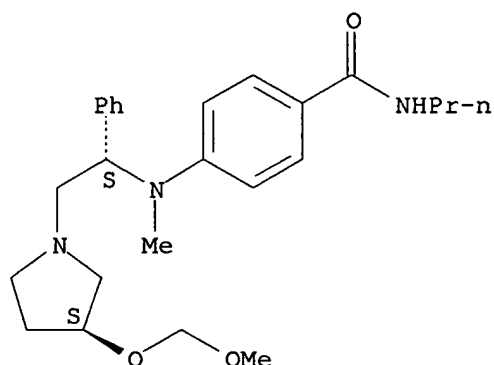
329365-45-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolidinyl- and pyrrolinylethylarylamines as kappa opioid receptor agonists)

RN 204970-95-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

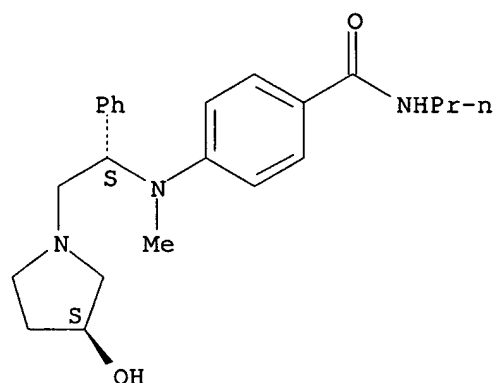
Absolute stereochemistry.



RN 204970-99-0 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

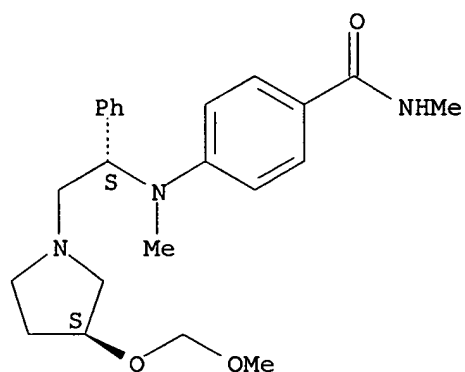


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RN 204971-01-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl- (9CI) (CA INDEX NAME)

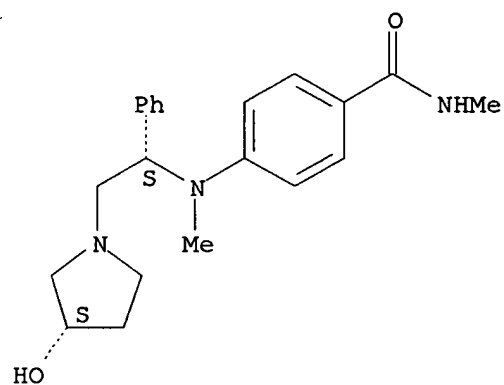
Absolute stereochemistry.



RN 204971-03-9 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl- (9CI) (CA INDEX NAME)

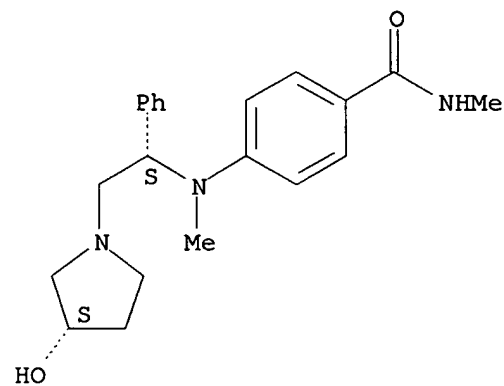
Absolute stereochemistry.



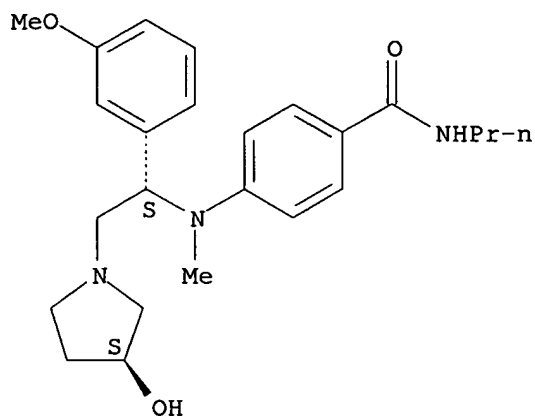
RN 204971-05-1 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

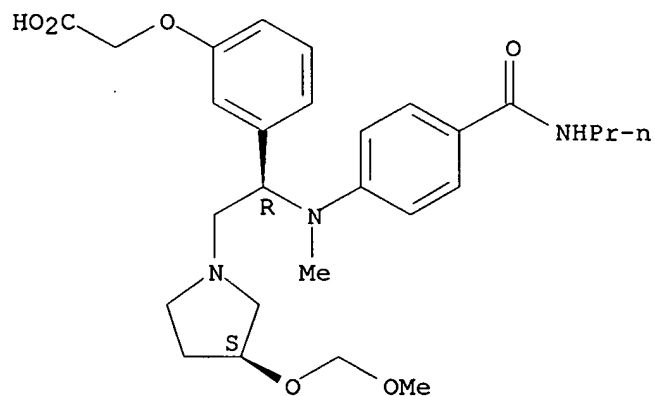


● HCl

RN 204973-57-9 CAPLUS

CN Acetic acid, [3-[2-[3-(methoxymethoxy)-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, [S-(R*,S*)]- (9CI)
(CA INDEX NAME)

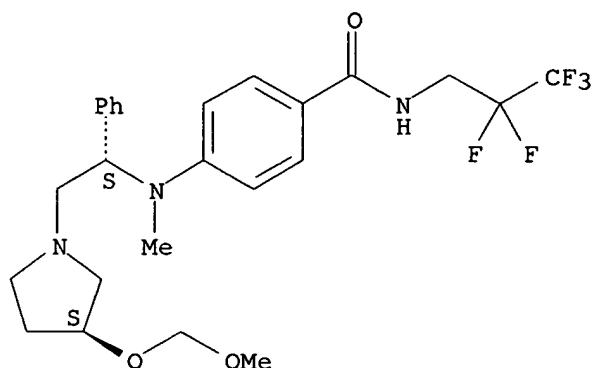
Absolute stereochemistry.



RN 204995-07-3 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil casreact

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
35.48	360.93

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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FILE CONTENT:1840 - 15 May 2005 VOL 142 ISS 20

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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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(FILE 'HOME' ENTERED AT 13:40:22 ON 20 MAY 2005)

FILE 'REGISTRY' ENTERED AT 13:40:29 ON 20 MAY 2005

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 0 S L1 FULL

FILE 'REGISTRY' ENTERED AT 13:44:38 ON 20 MAY 2005
L4 STRUCTURE UPLOADED
L5 7 S L4
L6 157 S L4 FULL

FILE 'CAPLUS' ENTERED AT 13:45:08 ON 20 MAY 2005
L7 7 S L6

FILE 'CASREACT' ENTERED AT 13:46:34 ON 20 MAY 2005

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3 L6
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14 COPPERS
14252 COPPER
(COPPER OR COPPERS)
2473 CUPROUS
1898 CUPRIC
L8 0 L7(L) (COPPER OR CUPROUS OR CUPRIC)

=> s L7 and copper
3 L6
14251 COPPER
14 COPPERS
14252 COPPER
(COPPER OR COPPERS)
L9 0 L7 AND COPPER

=> fil caplus

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

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SINCE FILE	TOTAL
ENTRY	SESSION
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FILE 'CAPLUS' ENTERED AT 13:48:18 ON 20 MAY 2005
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FILE COVERS 1907 - 20 May 2005 VOL 142 ISS 22
FILE LAST UPDATED: 19 May 2005 (20050519/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L7(L) (copper or cuprous or cupric)

CASREACT

843486 COPPER
423 COPPERS
843550 COPPER
(COPPER OR COPPERS)
19174 CUPROUS
27858 CUPRIC
L10 1 L7(L) (COPPER OR CUPROUS OR CUPRIC)

=> d L10

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:390231 CAPLUS

DN 140:391196

TI Process for the preparation of pyrrolidinyl ethylamine compounds via a copper-mediated aryl amination

IN Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel

PA Pfizer Products Inc., USA

SO PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004039785	A1	20040513	WO 2003-IB4676	20031022
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004152896	A1	20040805	US 2003-699106	20031031
PRAI	US 2002-423328P	P	20021101		
OS	MARPAT 140:391196				

=> s L7 and copper

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(COPPER OR COPPERS)

L11 1 L7 AND COPPER

=> d L11

L11 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

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 GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
 LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
 OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
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 PRAI US 2002-423328P P 20021101
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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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